

Resmetirom (MGL-3196)

CAS Registry No.: 920509-32-6

Formal Name: 2-(3,5-dichloro-4-((5-isopropyl-6-oxo-1,6-dihydropyridazin-3-yl)oxy)phenyl)-3,5-dioxo-2,3,4,5-tetrahydro-1,2,4-triazine-6-carbonitrile

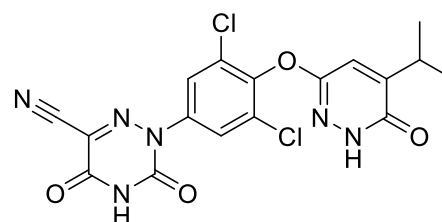
EUBOPEN ID: EUB0001081a

Molecular Formula: C₁₇H₁₂Cl₂N₆O₄

Molecular Weight: 435.22 g/mol

Smiles: CC(C)C1=CC(=NNC1=O)OC2=C(C=C(C=C2Cl)N3C(=O)NC(=O)C(=N3)C#N)Cl

Recommended concentration: 10 μM



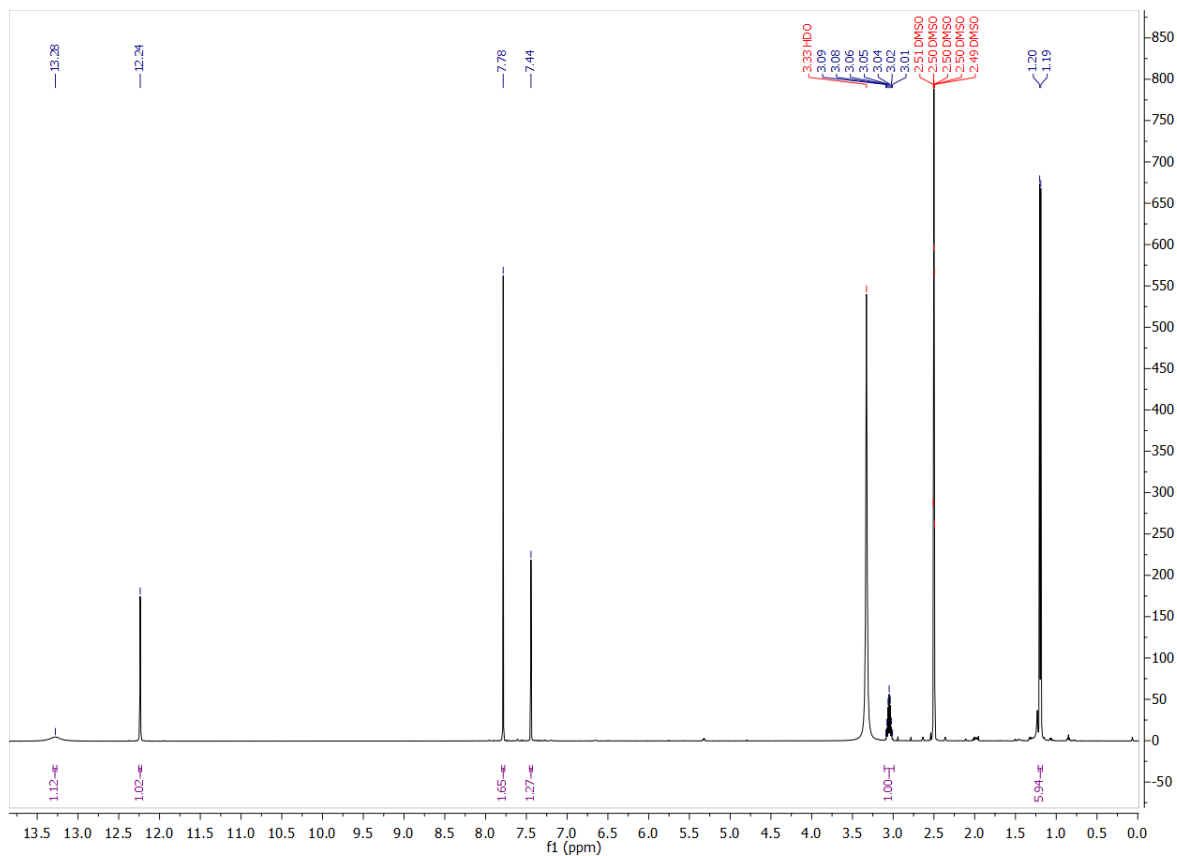
Biological activity

		Type	IC ₅₀ /EC ₅₀ [μM]	Reference
Main NR target:	NR1B2 (THRβ)	Agonist	0.2	https://doi.org/10.1021/jm4019299
NR off-target:				

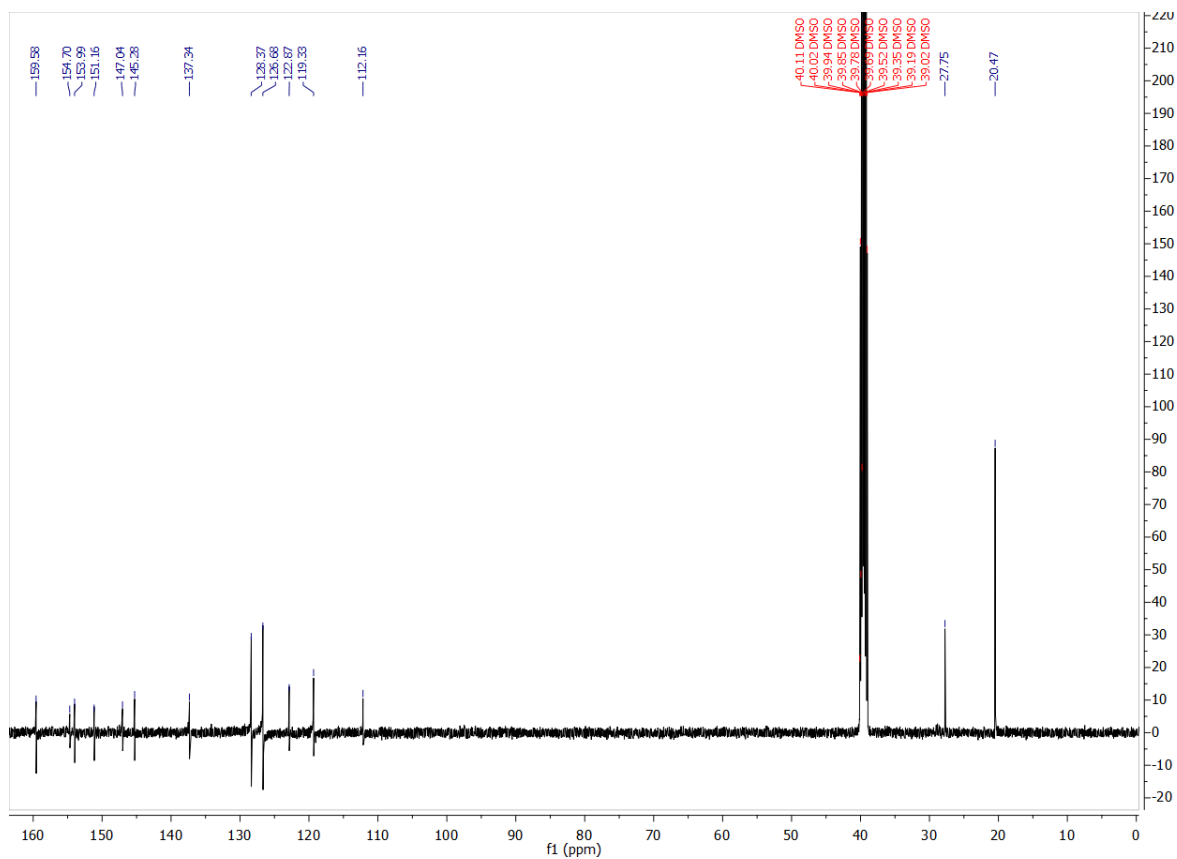
COMPOUND INFORMATION

Identity

¹H NMR



¹³C NMR



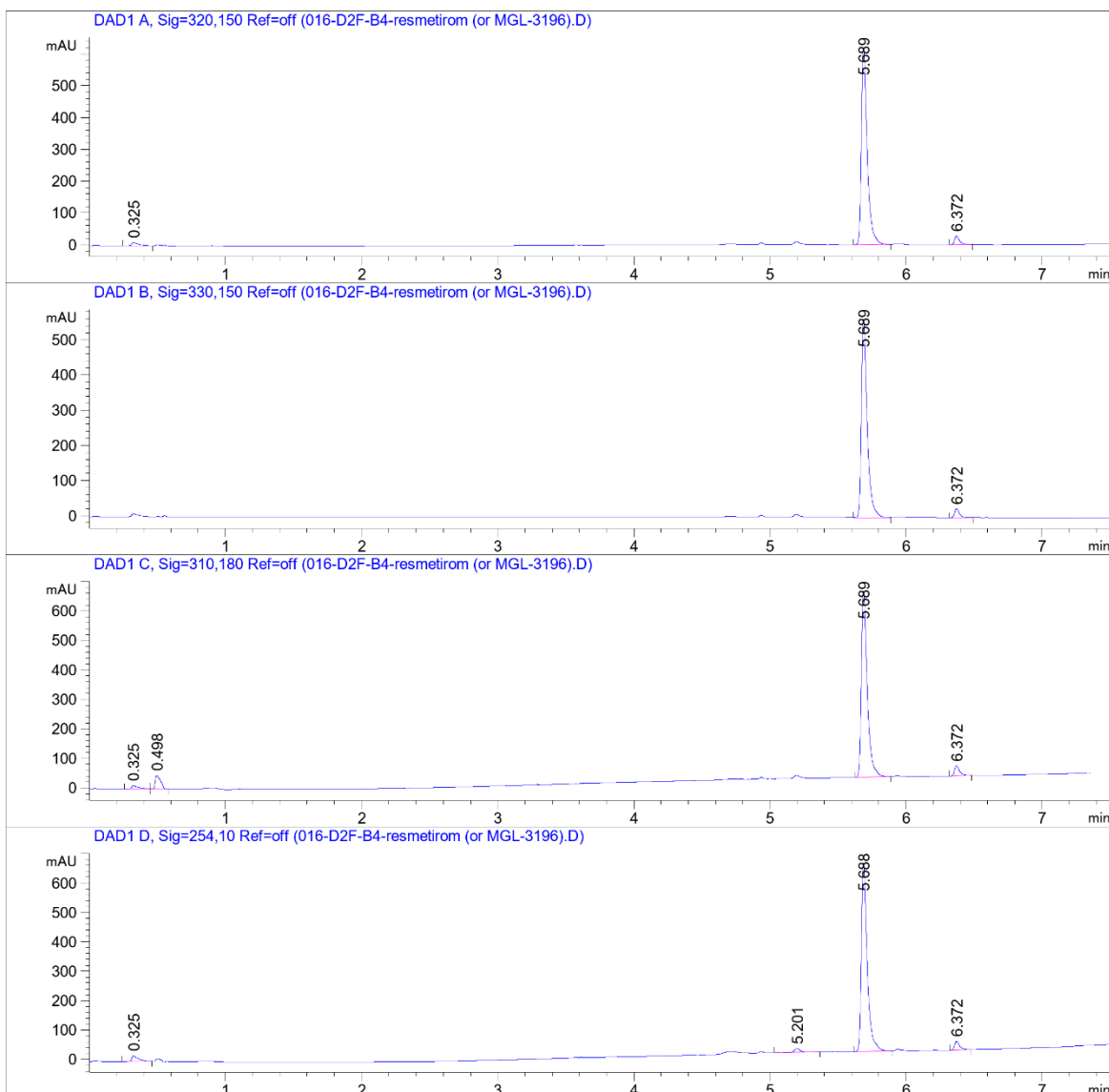
COMPOUND INFORMATION

Purity

Data File W:\analyti...irstPassB 2022-02-18 17-58-18\016-D2F-B4-resmetirom (or MGL-3196).D

Sample Name: resmetirom (or MGL-3196)

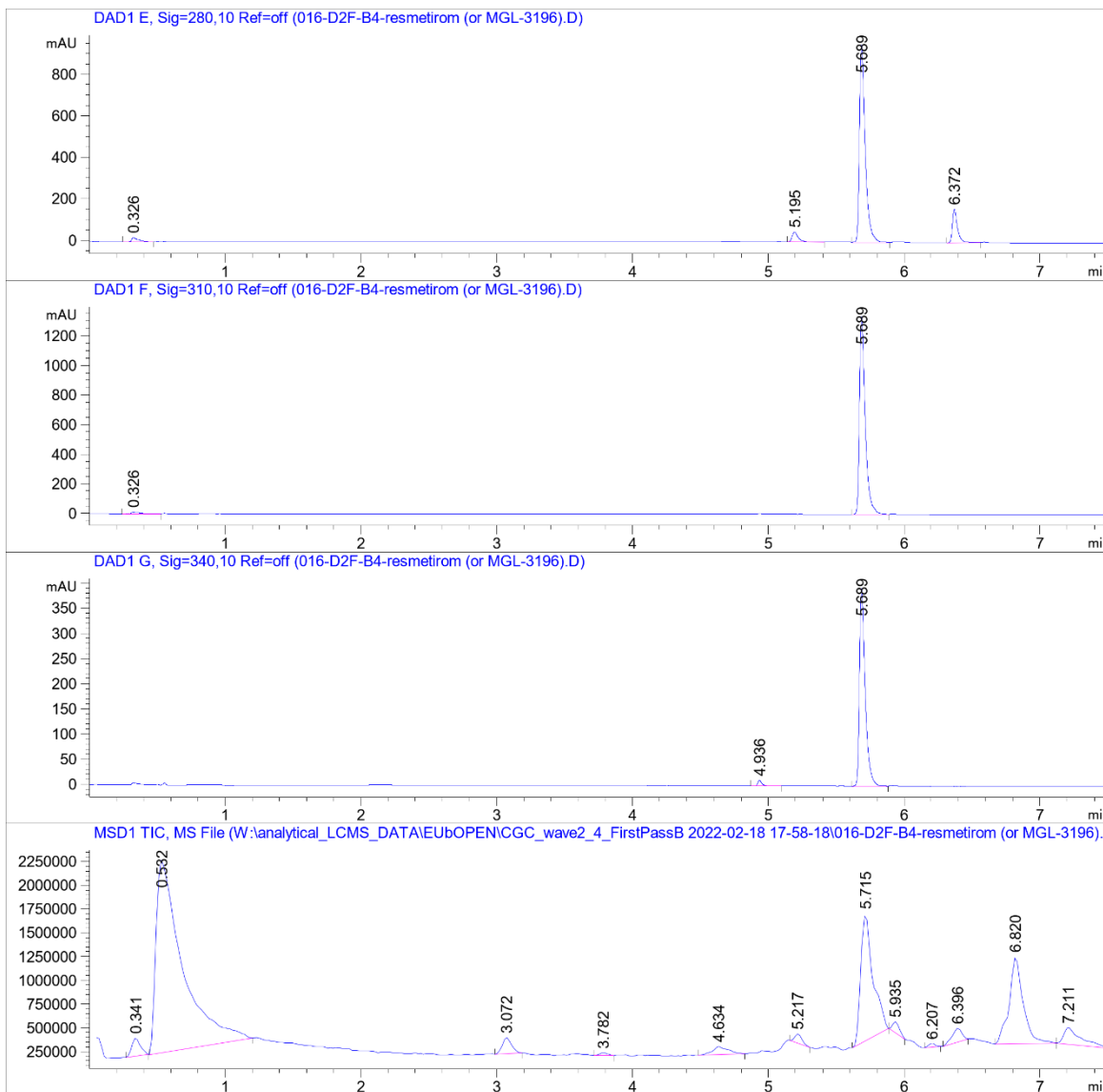
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=====
Acq. Operator   : SYSTEM                      Seq. Line :   16
Sample Operator : SYSTEM
Acq. Instrument : LCMS test                   Location  : D2F-B4
Injection Date  : 2/18/2022 8:47:01 PM       Inj       :    1
                                           Inj Volume: Inj prog
Sequence File   : W:\analytical_LCMS_DATA\EUBOPEN\CGC_wave2_4_FirstPassB 2022-02-18 17-58-18
                  \CGC_wave2_4_FirstPassB.S
Method          : W:\analytical_LCMS_DATA\EUBOPEN\CGC_wave2_4_FirstPassB 2022-02-18 17-58-18
                  \CGL_FIRSTPASS_GENERALMETHOD_VIAL1+2_20210319.M (Sequence Method)
Last changed    : 1/25/2022 4:36:18 PM by SYSTEM
Method Info     : CGL wellplate, 0.5 uL of 10 mM DMSO, general method
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COMPOUND INFORMATION

Data File W:\analyti...irstPassB 2022-02-18 17-58-18\016-D2F-B4-resmetirom (or MGL-3196).D

Sample Name: resmetirom (or MGL-3196)



COMPOUND INFORMATION

Data File W:\analyti...irstPassB 2022-02-18 17-58-18\016-D2F-B4-resmetirom (or MGL-3196).D

Sample Name: resmetirom (or MGL-3196)

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70, "POS Scan"

Spectra from peak tops.

Noise Cutoff: 1000 counts.

Reportable Ion Abundance: > 50%.

LC Signal: DAD1 A, Sig=320,150 Ref=off

Peak matching window: 0.1 min

Retention Time (LC)	LC Area	Retention Time (MS)	MS Area	Mol. Weight or Ion
0.325	37	0.341	822951	182.90 I 158.90 I 142.00 I
-	-	0.532	27432850	157.00 I
-	-	3.072	806655	239.10 I 217.10 I
-	-	3.782	129627	274.30 I
-	-	4.634	673506	332.20 I
-	-	5.217	370917	338.20 I 316.30 I 298.30 I
5.689	1835	5.715	8266391	437.00 I 435.00 I
-	-	5.935	415266	318.20 I 296.20 I 282.20 I 280.20 I
-	-	6.207	124596	228.20 I
6.372	71	6.396	713739	350.20 I 282.30 I 254.20 I 243.10 I
-	-	6.820	6471295	282.30 I
-	-	7.211	1498464	284.20 I 282.30 I

